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Study of Co-Existence of Superconductivity and Magnetism in Iron Pnictide Superconductors

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ABSTRACT

The effect of Antiferromagnetic order on superconducting order parameter (Δ) in Iron-pnictide superconductor has been studied by using double time retarded Green's Functions Technique, and expression for (Δ) has been obtained. The expression is found to be depending on the Antiferromagnetic order parameter (η) along with temperature (T). It has been found that at superconducting order parameter and antiferomgnetic order parameter decreasing with increasing temperature but superconducting order parameter (Δ) becomes almost zero at Transition Temperature. Results also shows that the Co-Existence of Magnetism and Superconductivity.

Keywords: Iron-pnictide, Antiferromagnetic order , Co-Existence, High Tc Superconductor

INTRODUCTION

After the discovery of high Tc cuprate superconductors in 1986[1] at 35 K, the field is buzzing with research activities. Efforts to increase the transition temperature are currently going on. Till now the highest reached Tc under pressure is 164 K in $HgBa_2Ca_2Cu_3O_{8+8}$[2]. These cuprates have unconventional properties both in normal and superconducting state[3-4]. Till date there is no consensus on the origin of pairing mechanism.

It is now widely suggested that spin – fluctuation driven pairing mechanism provides a good agreement between theory and experiments[5]. However, there are several experimental observations which clearly indicate that this purely electronic picture is incomplete and lattice effects have to be taken into acount[6-8].

In 2008 a new class of high TC superconductors LaFeAs(O, F) has found[9] with the remarkable T_C of 26 k. Similar to high- TC cuprates, the superconductivity in iron arsenide compounds is related to a layered structure. The electrical conductivity and magnetization measurements demonstrate that the F– ion-doped layered LaOFeAs is a bulk superconductor.

It has found[10] that the Characteristic normal-state charge transport in the oxygen-deficient iron-arsenides LnFeAsO1−y (Ln: La and Nd) with the highest TC's among known Fe-based superconductors. The effect of "doping" in this system is mainly on the carrier scattering, quite distinct from that in high- TC cuprates. In the superconducting regime of the La system with maximum T_C = 28 k, the low-temperature resistivity is dominated by a T^2 term. On the other hand, in the Nd system with T_C higher than 40 k, the carriers are subject to stronger scattering showing T -linear resistivity and small magnetoresistance. Such strong scattering appears crucial for high- T_C superconductivity in the iron-based system.

Recently scientists[11] have studied the magnetic excitations of undoped iron oxypnictides using a three-dimensional Heisenberg model with single-ion anisotropy. Analytic forms of the spin wave dispersion, velocities, and structure factor are given. Aside from quantitative comparisons which can be made to inelastic neutron scattering experiments, they also gave qualitative criteria which can distinguish various regimes of coupling strength. They reported that the magnetization reduction due to quantum zero point fluctuations shows clear dependence on the c-axis coupling.

MATERIAL AND METHODS

Mathematical Formulation:

In the present work double-time retarded Green's function technique given by Zubarev (1960) has been used as a mathematical tool. The Green's functions are the suitable simplification of the concept of correlation functions and work as a propagator. They are connected with the assessment of experimental quantities and have shown good advantages when equation are formulated and solved. Our Model Hamiltonian is:

$$H = \sum_{k\sigma} \epsilon_k a^+_{k\sigma} a_{k\sigma'} - V \sum_{kk'} a^+_{k\uparrow} a^+_{-k\downarrow} a_{-k'\downarrow} a_{k\uparrow} + \sum_{l\sigma} E_l a^+_{l\sigma} a_{l\sigma} + \left(\sum_{klm} G^{lm}_K a^+_{-k\uparrow} a^+_{k\downarrow} b_{l\uparrow} b_{m\downarrow} + h.c. \right) +$$

$$\sum_{lm\sigma\sigma'} J_{lm} b^+_{l\sigma} b^+_{m\sigma'} b_{l\sigma'} b_{m\sigma} \quad (1)$$

H = H1 +H2+H3+H4+H5

Where, 1: First (H1) term or energy of mobile (conduction) electrons, with $a^+_{k\sigma}$& $a_{k\sigma}$ are creation and annihilation operators of an electron having the wave vector k and the spin projection σ = $\uparrow$ or $\downarrow$ and ϵ_k representing the single particle energy of conduction electron.

2: Second (H2) term describe BCS types, where V are usual pairing interaction.

3:Third (H3) term represent $\epsilon_l$energy localized electron with $a^+_{l\sigma}$&$a_{l\sigma'}$ are creation and annihilation operators of an electron having the wave vector l and the spin projectionσ = $\uparrow$ or $\downarrow$

4:Forth (H4) term is the interaction term between conduction electrons and localized electrons due to some unspecified mechanism with effective interaction constant (G^{lm}_K).

5: Fifth (H5) term is the spin exchange interaction between localized electron and conduction electrons(J_{lm}) being the effective exchange constant.

We consider two Green Function'sfor conduction layers, which are define as:

$$G^{\uparrow\uparrow}_{qq} = \langle\langle a_{q\uparrow}, a^+_{-q\downarrow} \rangle\rangle \quad (2)$$

$$G^{\downarrow\uparrow}_{-qq} = \langle\langle a^+_{-q\downarrow} a^+_{q\uparrow} \rangle\rangle \quad (3)$$

We also use the equation of Fourier transform, which is

$$\omega G_{(\omega)} = \langle [A,B] \rangle + \langle\langle [A,H]; B \rangle\rangle$$

then the equation of motion in Fourier transform becomes

$$\omega G_{qq}^{\uparrow\uparrow} = \frac{1}{2\pi} + \langle\langle [a_{q\uparrow}, H]; a_{q\uparrow}^{+} \rangle\rangle$$

using model Hamiltonian equation (1) and Green's function defined by (2)&(3), we obtain the following two equation of motion :

$$(\omega - E_q) G_{qq}^{\uparrow\uparrow} = \frac{1}{2\pi} + (\Delta - \eta) G_{-qq}^{\downarrow\uparrow} \quad (4)$$

$$(\omega + E_q) G_{-qq}^{\downarrow\uparrow} = (\Delta - \eta) G_{qq}^{\uparrow\uparrow} \quad (5)$$

Here, $\eta = \sum_{lm} G_q^{lm} \langle a_{m\uparrow} a_{l\downarrow} \rangle$ and, $\Delta = \sum_q V \langle a_{-q\downarrow} + a_{q\uparrow} \rangle$

After solving equation (4) & (5), we get two Green's Functions:

$$G_{qq}^{\uparrow\uparrow} = \frac{(\omega + E_q)}{2\pi[(\omega^2 - E_q{}^2 + (\Delta - \eta)^2]} \quad (6)$$

$$G_{-qq}^{\downarrow\uparrow} = \frac{-(\Delta - \eta)}{2\pi[(\omega^2 - E_q{}^2 + (\Delta - \eta)^2]} \quad (7)$$

The correlation function related $\langle a_{-q\downarrow} a_{q\uparrow} \rangle$ is related to Green's function (3), as:

$$\langle a_{-q\downarrow} a_{q\uparrow} \rangle = i \int_{-\infty}^{\infty} \frac{[G_{-qq}^{\downarrow\uparrow}(\omega + i\varepsilon) - G_{-qq}^{\downarrow\uparrow}(\omega - i\varepsilon)]}{e^{\beta\omega} - 1} d\omega \quad (8)$$

After solving equation (7) & (8), we get the correlation function:

$$\langle a_{-q\downarrow} a_{q\uparrow} \rangle = \frac{(\Delta - \eta)}{2\sqrt{E_q^2 - (\Delta - \eta)^2}} \tanh \frac{\sqrt{E_q^2 - (\Delta - \eta)^2}}{2kT} \quad (9)$$

Here Δ = superconducting order parameter

η = magnetic order parameter.

The superconducting order Δ is related to this correlation function $\langle a_{-q\downarrow} a_{q\uparrow} \rangle$ as:

$$\Delta = \sum_q V \langle a_{-q\downarrow} a_{q\uparrow} \rangle \quad (10)$$

By putting the correlation function $\langle a_{-q\downarrow} a_{q\uparrow} \rangle$in this equation (10), we get the expression of superconducting order parameter Δ as:

$$\Delta = \sum_{qn} V \frac{(\Delta - \eta)}{2\sqrt{E_q^2 - (\Delta - \eta)^2}} \tanh \frac{\sqrt{E_q^2 - (\Delta - \eta)^2}}{2kT} \quad (11)$$

The sum may be changed into the integral by introducing the density of states.

$$N(\epsilon) = \frac{1}{V} \sum \rightarrow \frac{1}{2\pi^2} \int d^3 k = \int_{-E_f}^{\infty} dE N(E) \quad (12)$$

The summation with respect to q and n extends over all allowed pair states, therefore,

$$\Delta = 2 N(0) V \int_0^{\hbar\omega} dE \frac{(\Delta - \eta)}{2\sqrt{(\epsilon_q)^2 + (\Delta - \eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2 + (\Delta - \eta)^2}}{2} \quad (13)$$

Where $E^2 = (\epsilon_q)^2 + (\Delta - \eta)^2$

Let $N(0)V = \lambda$ Then

$$\frac{\Delta}{\lambda}=\int_0^{\hbar\omega} dE \frac{(\Delta-\eta)}{2\sqrt{(\epsilon_q)^2+(\Delta-\eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2+(\Delta-\eta)^2}}{2} \tag{14}$$

Let us study the equation in different case as

T→ok and T→ TC as T→ 0k

$$\beta = \infty \qquad (\beta=\frac{1}{kT})$$

One can take, $\tanh\frac{\beta E}{2} \to 1$

Then the above equation become as follows,

$$\frac{\Delta}{\lambda}=\int_0^{\hbar\omega} dE \frac{(\Delta-\eta)}{2\sqrt{(\epsilon_q)^2+(\Delta-\eta)^2}} \tag{15}$$

Using the integral $\int \frac{a}{\sqrt{a^2+x^2}}dx = a \arcsin\frac{x}{a}$

Then above equation become as,

$$\frac{1}{\lambda} = (1-\frac{\Delta}{\eta}) \arcsin\left(\frac{\hbar\omega}{(\Delta-\eta)}\right) \tag{16}$$

$$(1-\frac{\Delta}{\eta}) \arcsin\left(\frac{\hbar\omega}{\Delta-\eta}\right)=\left(1-\frac{\Delta}{\eta}\right)\ln[\frac{\hbar\omega}{(\Delta-\eta)}+\sqrt{\frac{(\hbar\omega)^2}{(\Delta-\eta)^2}}+1] \tag{17}$$

$$(1-\frac{\Delta}{\eta}) \arcsin\left(\frac{\hbar\omega}{\Delta-\eta}\right) \approx \left(1-\frac{\Delta}{\eta}\right)\ln[\frac{2\hbar\omega}{(\Delta-\eta)}] \tag{18}$$

$$(\Delta-\eta) = 2\hbar\omega \exp\frac{-1}{\lambda(1-\frac{\Delta}{\eta})} \tag{19}$$

The equation (19) similar to BCS theory except the η and $\left(1-\frac{\Delta}{\eta}\right)$ terms. We use $\Delta(0)$of BCS theory at T=0 is given by

$$2\Delta(0) = 3.5kBTC \tag{20}$$

for the compound SmFeAs$F_xO_{1-x}$the experimental result of TC= 51:5k , so that

$\Delta(0)$= 1.75kBTC=5.24063

At T = 0 the expression for η using equation (18) becomes

$$\eta= 1{:}75kBTC - 2\hbar\omega \exp\frac{-1}{\lambda(1-\frac{\eta}{1{:}75\, k_B T_c})} \tag{21}$$

As T→ TC using equation (14)

$$\frac{\Delta}{\lambda} = \int_0^{\hbar\omega} dE \frac{(\Delta-\eta)}{2\sqrt{(\epsilon_q)^2+(\Delta-\eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2+(\Delta-\eta)^2}}{2} \tag{22}$$

$$\frac{1}{\lambda} = \int_0^{\hbar\omega} dE \frac{(1-\frac{\eta}{\Delta})}{2\sqrt{(\epsilon_q)^2+(\Delta-\eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2+(\Delta-\eta)^2}}{2} \tag{23}$$

$$= \int_0^{\hbar\omega} dE \frac{1}{\sqrt{(\epsilon_q)^2+(\Delta-\eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2+(\Delta-\eta)^2}}{2} - \int_0^{\hbar\omega} dE \frac{\eta}{\Delta\sqrt{(\epsilon_q)^2+(\Delta-\eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2+(\Delta-\eta)^2}}{2} \tag{24}$$

At T=TC, $\Delta = 0$

The first integral of equation (24) becomes as

$$=\int_0^{\hbar\omega} dE \frac{1}{\sqrt{(\epsilon_q)^2 + (\eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2 + (\eta)^2}}{2} \text{then,}$$

$$= \int_0^{\hbar\omega} dE \frac{\tanh^{\beta\epsilon}/_2}{\epsilon} - \int_0^{\hbar\omega} dE\eta^2 \frac{4}{\beta} \Sigma_{n=0}^{\infty} \frac{1}{a^4 (1+x^2)} \quad (25)$$

After solving equation (25) we get following expression

$$= \ln 1.14 \frac{\hbar\omega}{k_B T_C} - \eta^2 (\frac{1}{\pi k_B T_C})^2 \frac{8.414}{8}$$

The second integral of equation of (24) applying l' Hospital's rule (differentiating the numerator and denominator) because Δ=0

$$I2 = \int_0^{\hbar\omega} dE \frac{\eta}{\Delta\sqrt{(\epsilon_q)^2 + (\Delta-\eta)^2}} \tanh \frac{\beta\sqrt{(\epsilon_q{}^2 + (\Delta-\eta)^2}}{2}$$

$$= \int_0^{\hbar\omega} dE\eta^2\beta \frac{(1-\tanh^2)\frac{\beta\sqrt{(\epsilon_q{}^2 + (\eta)^2}}{2}}{2(\epsilon_q{}^2 + (\eta)^2} \quad (26)$$

Combining the results equations (24) of first and the second integral result gives,

$$\frac{1}{\lambda} = \ln 1.14 \frac{\hbar\omega}{k_B T_C} - \eta^2 (\frac{1}{\pi k_B T_C})^2 \frac{8.414}{8} + \int_0^{\hbar\omega} dE\eta^2\beta \frac{(1-\tanh^2)\frac{\beta\sqrt{(\epsilon_q{}^2 + (\eta)^2}}{2}}{2(\epsilon_q{}^2 + (\eta)^2} \quad (27)$$

The third terms of equations (27) expanding which are two terms $\int_0^{\hbar\omega} dE\eta^2\beta \frac{(1-\tanh^2)\frac{\beta\sqrt{(\epsilon_q{}^2 + (\eta)^2}}{2}}{2(\epsilon_q{}^2 + (\eta)^2}$

$$= \int_0^{\hbar\omega} dE\eta^2\beta \frac{\left(\frac{\beta\sqrt{(\epsilon_q{}^2 + (\eta)^2}}{2}\right)}{2(\epsilon_q{}^2 + (\eta)^2} + \int_0^{\hbar\omega} dE\eta^2\beta \frac{\tanh^2 \frac{\beta\sqrt{(\epsilon_q{}^2 + (\eta)^2}}{2}}{2(\epsilon_q{}^2 + (\eta)^2}$$

$$\int_0^{\hbar\omega} dE\eta^2\beta \frac{(\frac{\beta\sqrt{(\epsilon_q{}^2 + (\eta)^2}}{2}}{2(\epsilon_q{}^2 + (\eta)^2} = \frac{\eta^2}{2k_B Tc} \arctan \frac{\hbar\omega}{\eta} = \frac{\eta}{4k_B Tc} \ln[\frac{\eta-\hbar\omega}{\eta+\hbar\omega}] \quad (28)$$

Substituting equation (28) in (27) and simplifying gives that

$$\frac{1}{\lambda} = \ln 1.14 \frac{\hbar\omega}{k_B T_C} - \eta^2 \left(\frac{1}{\pi k_B T_C}\right)^2 \frac{8.414}{8} + \frac{\eta}{4k_B T_C} \ln[\frac{\eta-\hbar\omega}{\eta+\hbar\omega}] \quad (29)$$

For small η we can ignore the η^2 term the equation (28) becomes,

$$\frac{1}{\lambda} = \ln 1.14 \frac{\hbar\omega}{k_B T_C} + \frac{\eta}{4k_B T_C} \ln[\frac{\eta-\hbar\omega}{\eta+\hbar\omega}] \quad (30)$$

$$k_B T_C = 1.14\exp -(\frac{1}{\lambda - a\eta}) \quad (31)$$

$$T_C = \frac{1.14\hbar\omega}{k_B} \exp -(\frac{1}{\lambda - a\eta})$$

Where, a= $\left(\frac{1}{4k_B T_C}\ln\left[\frac{\eta-\hbar\omega}{\eta+\hbar\omega}\right]\right)$

$\hbar\omega$= (0.002), $\lambda = 0.3 - 0.9, \eta = 0.05 - 7$, and a= 0.00000067

These values are taken from experimental data obtained by D. Dagher et al.

FOR LOCALIZED ELECTRONS:

Now, we introduce a Green's function for localized sites, defining as-

$$G_{11'}^{\uparrow\uparrow} = \langle\langle a_{l\uparrow},\ a_{l'\downarrow}^{+} \rangle\rangle \tag{32}$$

And writing equation of motion as-

$$\omega G_{11'}^{\uparrow\uparrow} = \frac{1}{2\pi} + \langle\langle [a_{l\uparrow},\ H], a_{l'\uparrow}^{+} \rangle\rangle \tag{33}$$

Now, evaluating the commutator $[a_{l'\uparrow}, H]$ using the Hamiltonian (1), we get the commutative relation:

$$[a_{l'\uparrow}, H] = E_{l'} a_{l'\uparrow} + \sum_m J_{l'm}\, a_{m\downarrow}^{+} a_{l'\downarrow} a_{m\uparrow} - \sum_l J_{l'l}\, a_{l\downarrow}^{+} a_{l\uparrow} a_{l'\downarrow} + \sum_{km} G_k^{l'm}\, a_{m\downarrow}^{+}\, a_{-k\downarrow} a_{-k\downarrow} a_{k\uparrow} \tag{34}$$

Putting the value in commutator $[a_{l'\uparrow}, H]$ equation (33)

$$\omega G_{l'l'}^{\uparrow\uparrow} = \frac{1}{2\pi} + E_{l'}\langle\langle a_{l'\uparrow}; a_{l'\uparrow}^{+}\rangle\rangle - \sum_{m'} J_{l'm'}\langle a_{m'\uparrow}; a_{l'\downarrow}\rangle\langle\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle\rangle - \sum_{m'} J_{m'l'}\langle a_{m'\uparrow}; a_{l'\downarrow}\rangle\langle\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle\rangle + \sum_{km'} G_k^{l'm'}\langle a_{-k\downarrow}; a_{k\uparrow}\rangle\langle\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle\rangle \tag{35}$$

Now we introduce the superconducting order parameter Δ_k and magnetic order parameter η for different localized site $\sum_k V\langle a_{-k\downarrow}; a_{k\uparrow}\rangle$ such as –

$$\Delta_k = \sum_k V\langle a_{-k\downarrow}; a_{k\uparrow}\rangle = \sum_k V\langle a_{k\uparrow}^{+}; a_{-k\downarrow}^{+}\rangle$$

$$\eta = G_k^{l'm'}\langle a_{m'\uparrow}; a_{l'\downarrow}\rangle = G_k^{l'm'}\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle$$

Substituting these order parameter in equation (35) , we obtain the equations:

$$\omega G_{11'}^{\uparrow\uparrow} = \frac{1}{2\pi} + E_{1'}\langle\langle a_{1'\uparrow}; a_{1'\uparrow}^{+}\rangle\rangle - \sum_{m'}\frac{J_{1'm'}}{G_k^{l'm'}}\sum_{m'}\frac{J_{1'm'}}{G_k^{l'm'}}\eta\langle\langle a_{m'\downarrow}^{+}; a_{1'\uparrow}^{+}\rangle\rangle + \sum_{km'}\frac{G_k^{l'm'}}{V}\Delta_k\langle\langle a_{m'\downarrow}^{+}; a_{1'\uparrow}^{+}\rangle\rangle \tag{36}$$

Now introducing other Green's Functions;

$$G_{l'l'}^{\downarrow\uparrow} = \langle\langle a_{l'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle\rangle \tag{37}$$

$$G_{m'l'}^{\downarrow\uparrow} = \langle\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle\rangle \tag{38}$$

$$G_{1'm'}^{\uparrow\uparrow} = \langle\langle a_{m'\uparrow}; a_{l'\uparrow}^{+}\rangle\rangle \tag{39}$$

Substituting these Green Function's inn equation (36), we get –

$$\omega G_{11'}^{\uparrow\uparrow} = \frac{1}{2\pi} + E_{1'} G_{11'}^{\downarrow\uparrow} - 2\sum_{m'}\frac{J_{1'm'}}{G_k^{l'm'}}\eta G_{m1'}^{\downarrow\uparrow} + \sum_{km'}\frac{G_k^{l'm'}}{V}\Delta_k G_{m1'}^{\downarrow\uparrow} \tag{40}$$

By taking Fourier transformation of equation (36) and after solving, finally we get the equation:

$$(\omega - E_{l'})G_{1'1'}^{\uparrow\uparrow} = \frac{1}{2\pi} + (\Delta_l - \eta_l)G_{m'l'}^{\downarrow\uparrow} \tag{41}$$

Where, $\Delta_l = \frac{G_k^{l'm'}}{V}\Delta$ and $\eta_l = 2\frac{J_{l'm'}}{G_k^{l'm'}}\eta$

The Green's Functions (37) may be written in term of equation of motions as:

$$\omega G_{l'l'}^{\downarrow\uparrow} = \langle\langle [a_{l'\downarrow}^{+}, H]; a_{l'\uparrow}^{+}\rangle\rangle \tag{42}$$

Now, evaluating the commutator $[a_{l'\downarrow}^{+}, H]$ using the Hamiltonian (1), we get:

$$[a_{l'\downarrow}^{+}, H] = -E_{l'}a_{l'\downarrow} + \sum_{m'} J_{l'm} a_{l'\uparrow}^{+} a_{m'\downarrow}^{+} a_{m'\uparrow} - \sum_{m'} J_{m'l} a_{m'\downarrow}^{+} a_{l'\downarrow}^{+} a_{m'\uparrow} + \sum_{km} G_k^{l'm} a_{k\downarrow}^{+} a_{-k\uparrow}^{+} a_{m'\uparrow}$$

Putting the value of commutator $[a_{l'\downarrow}^{+}, H]$ in the equation (42) we get-

$$[a_{l'\downarrow}^{+}, H] = -E_{l'}\langle\langle a_{l'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle\rangle - 2\sum_{m'} J_{l'm'}\langle a_{m'\downarrow}^{+}; a_{l'\uparrow}^{+}\rangle\langle\langle a_{m'\uparrow}; a_{l'\uparrow}^{+}\rangle\rangle + \sum_{km'} G_k^{l'm'}\langle a_{k\uparrow}^{+}; a_{-k\downarrow}^{+}\rangle\langle\langle a_{m'\uparrow}; a_{l'\uparrow}^{+}\rangle\rangle \tag{43}$$

By substituting the order parameters in equations (43) we obtain the expression:

$$\omega G_{l'l'}^{\downarrow\uparrow} = -E_{l'}G_{l'l'}^{\downarrow\uparrow} - 2\sum_{m'} \frac{J_{l'm'}}{G_k^{l'm'}}\eta G_{m'l'}^{\uparrow\uparrow} + \sum_{km'} \frac{G_k^{l'm'}}{V}\Delta_k G_{m'l'}^{\uparrow\uparrow} \tag{44}$$

By taking Fourier transformation of equation (43) and after solving we get the equation:

$$(\omega + E_{l'})G_{l'l'}^{\downarrow\uparrow} = (\Delta_l - \eta_l)G_{m'l'}^{\uparrow\uparrow} \tag{45}$$

Now taking Green's Function (39) and written in terms of equation of motion as:

$$\omega G_{m'l'}^{\uparrow\uparrow} = \langle\langle [a_{m'\uparrow}^{+}, H]; a_{l'\uparrow}^{+}\rangle\rangle \tag{46}$$

Now, evaluating the commutator $[a_{m'\uparrow}^{+}, H]$ using the Hamiltonian (1), we get -

$$[a_{m'\uparrow}^{+}, H] = E_{m'}a_{m'\uparrow} - 2\sum_{m'} J_{m'l} a_{l'\downarrow}^{+} a_{l'\uparrow} a_{m'\uparrow} + \sum_{km} G_k^{l'm} a_{l'\downarrow}^{+} a_{-k\downarrow} a_{k\uparrow} \tag{47}$$

Putting the value of commutator $[a_{m'\uparrow}^{+}, H]$ in the equation (46), we get,

$$\omega G_{m'l'}^{\uparrow\uparrow} = -E_{l'}G_{m'l'}^{\uparrow\uparrow} - 2\sum_{m'} \frac{J_{l'm'}}{G_k^{l'm'}}\eta G_{l'l'}^{\downarrow\uparrow} + \sum_{km'} \frac{G_k^{l'm'}}{V}\Delta_k G_{l'l'}^{\downarrow\uparrow} \tag{48}$$

By taking Fourier transformation of equation (46) and after solving we get the equation;

$$(\omega - E_{m'})G_{m'l'}^{\uparrow\uparrow} = (\Delta_l - \eta_l)G_{l'l'}^{\downarrow\uparrow} \tag{49}$$

Now taking Green's Function (38) and written in terms of equation of motion as:

$$\omega G_{m'l'}^{\downarrow\uparrow} = \langle\langle [a_{m'\downarrow}^{+}, H]; a_{l'\uparrow}^{+}\rangle\rangle \tag{50}$$

Now, evaluating the commutator $[a_{m'\downarrow}^{+}, H]$ using the Hamiltonian (1), we get -

$$[a_{m'\downarrow}^{+}, H] = -E_{m'}a_{m'\downarrow} - 2\sum_{l'} J_{m'l'} a_{l'\downarrow}^{+} a_{m'\uparrow}^{+} a_{m'\uparrow} + \sum_{km} G_k^{l'm} a_{k\uparrow}^{+} a_{-k\downarrow}^{+} a_{l\uparrow} \tag{51}$$

Putting the value of commutator $[a_{m'\downarrow}^{+}, H]$ in the equation (50), we get,

$$\omega G_{m'l'}^{\downarrow\uparrow} = -E_{m'}G_{m'l'}^{\downarrow\uparrow} - 2\sum_{m'} \frac{J_{l'm'}}{G_k^{l'm'}}\eta G_{l'l'}^{\uparrow\uparrow} + \sum_{km'} \frac{G_k^{l'm'}}{V}\Delta_k G_{l'l'}^{\uparrow\uparrow} \tag{52}$$

By taking Fourier transformation of equation (50) and after solving we get the equation:

$$(\omega + E_{m'})G_{m'l'}^{\downarrow\uparrow} = (\Delta_l - \eta_l)G_{l'l'}^{\uparrow\uparrow} \tag{53}$$

So, finally four equation are obtained containing four Green's Functions:

$$(\omega - E_{l'})G^{\uparrow\uparrow}_{l'l'} = \frac{1}{2\pi} + (\Delta_l - \eta_l)G^{\downarrow\uparrow}_{m'l'}$$

$$(\omega + E_{l'})G^{\downarrow\uparrow}_{l'l'} = (\Delta_l - \eta_l)G^{\uparrow\uparrow}_{m'l'}$$

$$(\omega - E_{m'})G^{\uparrow\uparrow}_{m'l'} = (\Delta_l - \eta_l)G^{\downarrow\uparrow}_{l'l'}$$

$$(\omega + E_{m'})G^{\downarrow\uparrow}_{m'l'} = (\Delta_l - \eta_l)G^{\uparrow\uparrow}_{l'l'}$$

After solving these equations, we can Green's Functions $G^{\downarrow\uparrow}_{m'l'}$ as ;

$$G^{\downarrow\uparrow}_{m'l'} = \frac{(\Delta_l - \eta_l)}{2\pi\{\omega^2 - \epsilon^2 + (\Delta_l - \eta_l)^2\}} \tag{54}$$

Here magnetic order parameter,

$$\eta = \sum_{lm} G^{lm}_{q} \langle a_{m\uparrow} a_{l\downarrow} \rangle \tag{55}$$

Here correlation function $\langle a^{+}_{m'\downarrow}, a^{+}_{l'\uparrow} \rangle$ may be defined as

$$\langle a^{+}_{m'\downarrow}, a^{+}_{l'\uparrow} \rangle = i \int_{-\infty}^{\infty} \frac{[G^{\downarrow\uparrow}_{qq}(\omega + i\varepsilon) - G^{\downarrow\uparrow}_{qq}(\omega - i\varepsilon)]}{e^{\beta\omega} - 1} d\omega \tag{56}$$

After solving the Green's Functions (54) and putting in the equation (56), we get

$$\eta = \sum_{kl'} G^{l'm'}_{k} \frac{(\Delta_l - \eta_l)}{\sqrt{\epsilon^2 + (\Delta_l - \eta_l)^2}} \tanh \frac{\sqrt{\epsilon^2 + (\Delta_l - \eta_l)^2}}{2kT} \tag{57}$$

Sum changed into the integral by introducing density of states

$$\eta = 2\, N(0) G^{l'm'}_{k} \beta \int_0^{\hbar\omega} dE\, (\Delta_l - \eta_l) \frac{1}{2\beta E} \tanh \frac{\beta E}{2} \tag{58}$$

$E^2 = \epsilon^2 + (\Delta_l - \eta_l)^2$ And $\lambda_l = N(0) G^{l'm'}_{k}$

Applying same technique as in (22)the above equation at low temperature yields

$$\eta = \lambda_l P \ln(1.14 \frac{\hbar\omega}{k_B T}) + P^2 \left(\frac{1}{\pi k_B T_C}\right)^2 \tag{59}$$

Since $P^2 (= (\Delta_l - \eta_l)^2)$ is very small we can ignore the second term

$$\eta = \lambda_l P \ln\left(1.14 \frac{\hbar\omega}{k_B T}\right)$$

$$\eta = \lambda_l \ln(\Delta_l - \eta_l)(1.14 \frac{\hbar\omega}{k_B T}) \tag{60}$$

This implies that

$k_B T = 1.14\, \hbar\omega \exp \frac{(\eta)}{\lambda_l(\Delta_l - \eta_l)}$

$$T = T = \frac{1.14\hbar\omega}{k_B} \exp \frac{(\eta)}{\lambda_l(\Delta_l - \eta_l)} \tag{61}$$

Δ_l $\Delta_l = \frac{G^{l'm'}_{k}}{V} \Delta$, $\eta_l = 2 \frac{J_{l'm'}}{G^{l'm'}_{k}} \eta$ and

(Δ= superconducting order parameter and η= magnetic order parameter)

RESULTS AND DISCUSSION

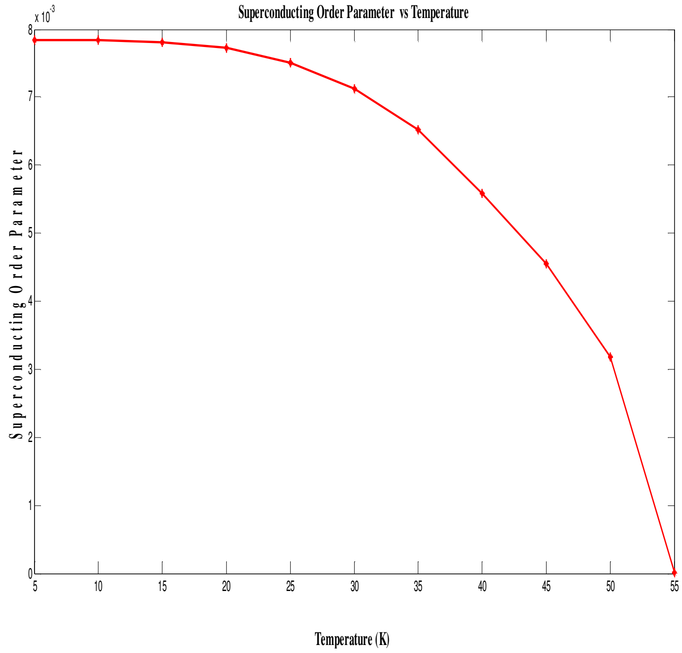

Fig 1.1 Variation of SC order parameter with Temperature (K)

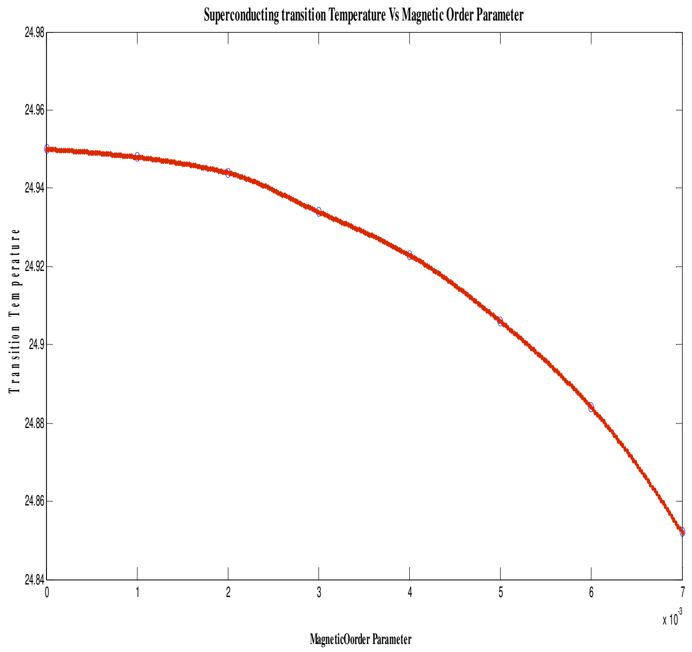

Fig 1.2 Variation of SC Transition Temperature (TC) With Magnetic Order Parameter (η)

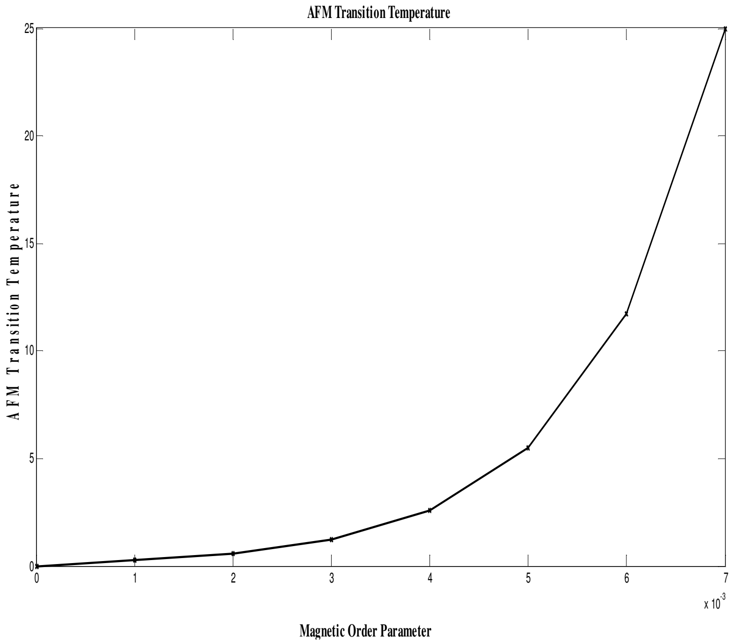

Fig1.3 Variation of AFM Temperature (Tm) With Magnetic Order Parameter (η)

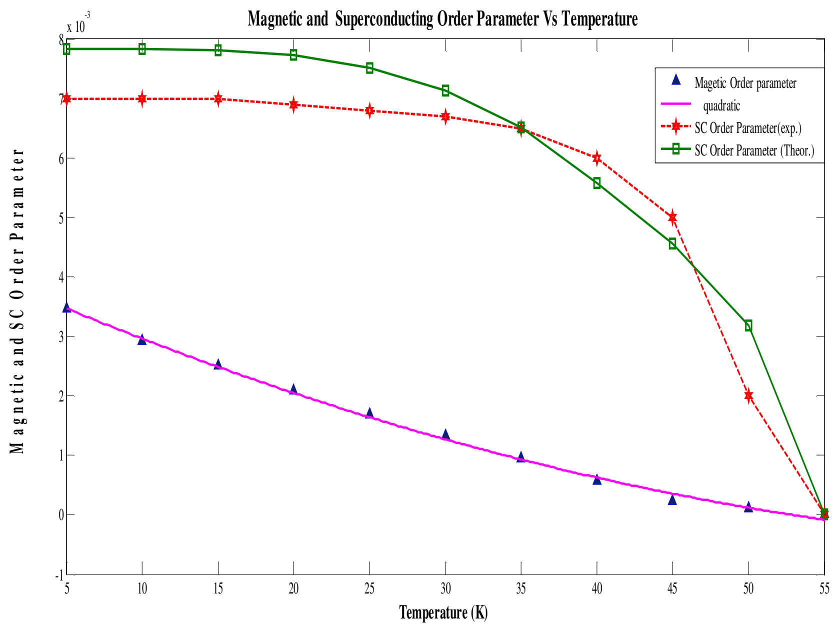

Fig1.4 Variation of Temperature (T) with SC Order Parameter Δ (Experimental) & SC Order parameter Δ (Theoretical) and Magnetic Order Parameter η.

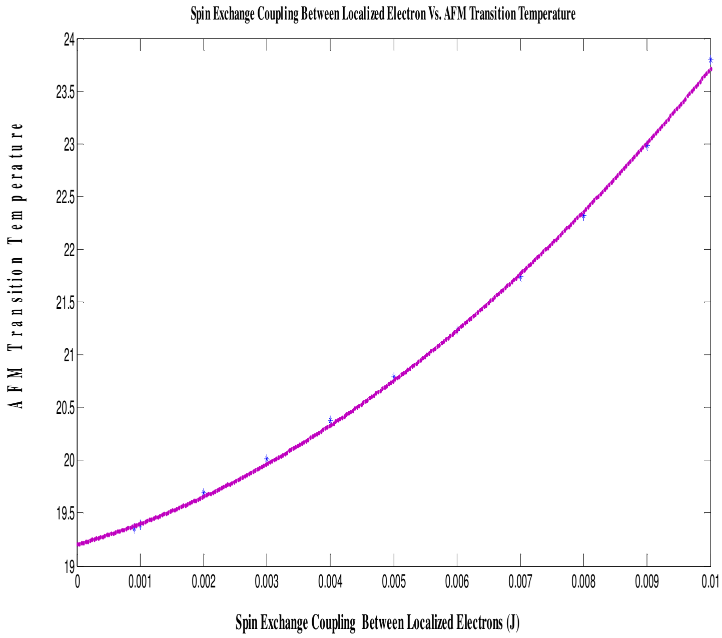

Fig 1.5 Variation of Spin Exchange Coupling Between Localized Electrons (J) with AFM Transition Temperature (Tm)

In the results the effect of temperature (T) on superconducting order parameter Δ has been described. We examined the effect of magnetic order parameter η on superconducting transition temperature (T) and on AFM transition temperature (Tm) in $SmO_{1-x}F_xFeAs$.,

To analyze co-existence region of SC order parameter and magnetic order parameter.

To analyze the role of spin exchange coupling (J) between localized electrons in the superconducting state.

In chapter three, using the model of the Hamiltonian and retarded double time temperature dependent Greens function formalism, we obtained mathematical expressions for superconducting critical temperature TC, the superconducting order parameter Δ the magnetic order parameter η and AFM transition temperature (Tm).

We plot the phase diagram of Δ versus T (K) which is shown in Figure 4.1 As seen in this figure, when the temperature increases the superconducting order parameter decreases and vanishes as the temperature is equal to the Transition temperature (TC) Based on Equations (64).

We plotted the phase diagram of TC versus η (Fig 4.2). This figure indicates, as the magnetic order parameter (η) increases the superconducting transition temperature TC decreases.

The phase diagram of magnetic ordering temperature(Tm) versus magnetic ordering (η) also plotted (Fig 4.3) based on the Equations (65). As we observed from this graph the magnetic transition temperature is increasing (directly proportional) as the magnetic order parameter increases.

The phase diagram of SC order parameter (as per BCS Theory experimental data reported by Y. Wang et al.)& SC order parameter (theoretically obtained by equation-64) Δ and Magnetic Order Parameter η versus Temperature, plotted (4.4) the common area of graph shows the co-existence region of η & Δ.

The phase diagram of spin exchange coupling (J) between localized electrons versus critical temperature (TC) plotted in (fig4.5) based on equations (65). To analyze the role of spin exchange coupling (J) between localized electrons in superconducting state (fig4.5) shows that with increase in spin exchange coupling, the TC first sharply increase and at higher value of J, this rate of increase TC is slow down with J.

CONCLUSION

In conclusion we can say that :

(a) As temperature increases superconducting order parameter decreases.

(b) When magnetic order parameter increases the critical temperature decreases.

(c) While the magnetic order parameter increases with the AFM transitional temperature.

(d) The phase diagram of SC order parameter (as per BCS Theory experimental data reported by Y. Wang et al.) & SC order parameter (theoretical) Δ and Magnetic Order Parameter η vs. Temperature, common area of graph shows that co-existence region of η & Δ. Behaviour of both, SC order parameter Δ & magnetic order parameter η with decreases with increases Temperature, Δ & η are behaves in same way with temperature. This indicates they are helping to each other.

(e) The expression η_l is found to dependent on the exchange interaction of localized electrons (J) and interaction of localized & conduction electron (G_k^{lm}) . Result show that initially as shows that with increase in spin exchange coupling, the T_C first sharply increase and higher value J, T_C reached at saturated value because the system is in pair state characterized by the fact that all electron locally paired.

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